

Extension of the 1D Four-Group Analytic Nodal Method to Full Multigroup

International Conference on Reactor Physics, Nuclear Power: A Sustainable Resource

B. D. Ganapol
D. W. Nigg

September 2008

The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance



This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint should not be cited or reproduced without permission of the author. This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights. The views expressed in this paper are not necessarily those of the United States Government or the sponsoring agency.

Extension of the 1D four-group analytic nodal method to full multigroup

B. D. Ganapol^{a,*} and D. W. Nigg^b

^a*Department of Aerospace and Mechanical Engineering, University of Arizona, Tucson AZ, USA*

^b*INL, Idaho Falls, ID, USA*

Abstract

In the mid 80's, a four-group/two-region, entirely analytical 1D nodal benchmark appeared. It was readily acknowledged that this special case was as far as one could go in terms of group number and still achieve an analytical solution. In this work, we show that by decomposing the solution to the multigroup diffusion equation into homogeneous and particular solutions, extension to any number of groups is a relatively straightforward exercise using the mathematics of linear algebra.

1. Introduction

Twenty-two years ago, a four-group/two-region, 1D analytic nodal benchmark first appeared [Parsons, Nigg, 1985(1),1985(2)] as an outgrowth of work supporting the TRAC-BD1 coupled core thermal hydraulics code [Aburomia, 1981]. While this represented an evolution beyond the two-group analytic formulation [Shober, 1978, Smith, 1979], it was readily apparent from the manipulations involved that following the same procedure for an arbitrary number of groups would not be possible. In their four-group formulation, Nigg and Parsons derived the complete analytical solution by removing all complex arithmetic. We shall show that by decomposing the solution into homogeneous

and particular solutions, extension to the multigroup case is a straightforward mathematical exercise. In particular, the solution closely resembles that of the one-group formulation.

The basics of this approach has previously appeared in the literature [Muller, 1989] but not in consistent mathematical way presented here. In particular, we formulate the multigroup solution similarly to a one-group solution through a modal analysis.

2. The Theory

2.1. Preliminaries

We begin with the multigroup diffusion equation in one-dimension given by Eq.(1). This

* Corresponding author bganapol@utk.edu

Tel: 865/974-0892; Fax: 865/974-0668.

equation describes the steady state diffusion of neutrons in a homogeneous region j and in group g .

$$\begin{aligned} & \left[D_{gj} \frac{d^2}{dx^2} - \Sigma_{gj} \right] \phi_{gj}(x) + \\ & + \chi_g \sum_{g'=1}^G \nu \Sigma_{fg'j} \phi_{g'j}(x) + \\ & + \sum_{g'=1}^G \Sigma_{gg'j} \phi_{g'j}(x) = -Q_{gj}(x). \end{aligned} \quad (1)$$

Here, $1 \leq j \leq n$, $1 \leq g \leq G$ and $x_{j-1} \leq x \leq x_j$.

In vector form, Eq.(1) becomes

$$\mathbf{M}_{jG}(x) \boldsymbol{\phi}_j(x) = -\mathbf{q}_j(x) \quad (2a)$$

where

$$\mathbf{M}_{jG}(x) \equiv \frac{d^2}{dx^2} \mathbf{I} + \boldsymbol{\gamma}_j \quad (2b)$$

with

$$\boldsymbol{\gamma}_j \equiv \begin{bmatrix} \gamma_{11} & \gamma_{12} & \cdots & \gamma_{1G} \\ \gamma_{21} & \cdots & & \cdots \\ \cdots & & & \cdots \\ \gamma_{G1} & \cdots & & \gamma_{GG} \end{bmatrix}, \quad (2c)$$

whose elements are

$$\begin{aligned} \gamma_{gg} & \equiv \frac{\chi_g \nu \Sigma_{fg} - (\Sigma_g - \Sigma_{gg})}{D_g} \\ \gamma_{gg'} & \equiv \frac{\chi_g \nu \Sigma_{fg'} + \Sigma_{gg'}}{D_g}, \quad g \neq g'. \end{aligned} \quad (2d)$$

Note that boldface type has been used for both vectors and matrices alike with the intended meaning to be obtained from context.

The flux and source group vectors are

$$\boldsymbol{\phi}_j(x) \equiv \{\phi_{gj}, g = 1, \dots, G\} \quad (2e)$$

$$\mathbf{q}_j(x) \equiv \{Q_{gj}(x)/D_{gj}, g = 1, \dots, G\}. \quad (2f)$$

In the usual way, we decompose the general solution into homogeneous and particular solutions

$$\boldsymbol{\phi}_j(x) = \boldsymbol{\Psi}_j(x) + \boldsymbol{\phi}_{pj}(x), \quad (3a)$$

where $\boldsymbol{\Psi}_j(x)$ is the solution to

$$\mathbf{M}_{jG}(x) \boldsymbol{\Psi}_j(x) = \mathbf{0}; \quad (3b)$$

and $\boldsymbol{\phi}_{pj}(x)$ solves

$$\mathbf{M}_{jG}(x) \boldsymbol{\phi}_{pj}(x) = -\mathbf{q}_j(x). \quad (3c)$$

We then apply the boundary conditions on the free surfaces x_0 and x_n and the internal interfaces to obtain the general solution.

3. General solution representation

3.1. The homogeneous solution

A straightforward treatment of the homogeneous equation requires the solution in terms of the eigenvalues B_j^2 and eigenfunctions $\boldsymbol{\Psi}_j$ of the diffusion operator by region

$$\left[\nabla^2 + B_j^2 \mathbf{I} \right] \boldsymbol{\Psi}_j(x) = \mathbf{0}, \quad (4)$$

where the ∇^2 is $\frac{d^2}{dx^2} \mathbf{I}$. When we introduce Eq.(4)

into Eq.(3b), the following homogeneous algebraic system results:

$$(\boldsymbol{\gamma}_j - B_j^2 \mathbf{I}) \boldsymbol{\Psi}_j(x) = \mathbf{0}, \quad (5a)$$

where the eigenvalues, B_{jk}^2 , $k = 1, 2, \dots, G$, are simply the eigenvectors of the $\boldsymbol{\gamma}_j$ -matrix

$$\text{Det}[\gamma_j - B_j^2 \mathbf{I}] = 0. \quad (5b)$$

For each k -mode therefore

$$\left[\frac{d^2}{dx^2} + B_{jk}^2 \right] \Psi_{jk}(x) = 0, \quad (6a)$$

yielding the general solution

$$\Psi_{gj}(x) = \sum_{k=1}^G \left[C_{jgk}^+ h_{jk}^+(x) + C_{jgk}^- h_{jk}^-(x) \right], \quad (6b)$$

where h_{jk}^\pm satisfies

$$\left[\frac{d^2}{dx^2} + B_{jk}^2 \right] h_{jk}^\pm(x) = 0. \quad (7a)$$

The most convenient boundary conditions for h_{jk}^\pm are

$$\begin{aligned} h_{jk}^+(x_j) &\equiv 1 & h_{jk}^-(x_j) &\equiv 0 \\ h_{jk}^+(x_{j-1}) &\equiv 0 & h_{jk}^-(x_{j-1}) &\equiv 1 \end{aligned} \quad (7b)$$

implying

$$\begin{aligned} h_{jk}^+(x) &= \left[\frac{\sin(B_{jk}(x - x_{j-1}))}{\sin(B_{jk}\Delta_j)} \right] \\ h_{jk}^-(x) &= \left[\frac{\sin(B_{jk}(x_j - x))}{\sin(B_{jk}\Delta_j)} \right], \end{aligned} \quad (7c)$$

where $\Delta_j \equiv x_j - x_{j-1}$. Note that the above expressions are also appropriate for complex B_{jk} .

The next task is to determine the coefficients C_{jgk}^\pm shown to satisfy

$$B_{jk}^2 C_{jgk}^\pm - \sum_{g'=1}^G \gamma_{gg'} C_{jg'k}^\pm = 0, \quad k=1, 2, \dots, G, \quad (8a)$$

and are the eigenvectors of the γ_j -matrix. Thus, there is a one-parameter family of solutions expressed in terms of an arbitrary constant vector. We choose that vector to be for the first group and therefore write for $g=2, 3, \dots, G$

$$C_{jgk}^\pm = \alpha_{gk} C_{j1k}^\pm \quad (8b)$$

Consistency requires $\alpha_{1k} \equiv 1$ (or 0) for $k=1, 2, \dots, G$ and Eq.(8a) gives

$$\sum_{g'=2}^G \left[B_{jk}^2 \delta_{gg'} - \gamma_{gg'} \right] \alpha_{g'k} = \gamma_{g1} \quad (8c)$$

for $g=2, 3, \dots, G, k=1, 2, \dots, G$. A region without fission or upscattering requires special consideration.

At this point, the representation of the homogeneous solution by group is

$$\Psi_{gj}(x) = \sum_{k=1}^G \left[\alpha_{gk} h_{jk}^+(x) C_{j1k}^+ + \alpha_{gk} h_{jk}^-(x) C_{j1k}^- \right],$$

or in the more convenient vector form

$$\begin{aligned} \Psi_j(x) &= \alpha_j h_j^+(x) C_{j1}^+ + \\ &\quad + \alpha_j h_j^-(x) C_{j1}^- \end{aligned} \quad (9a)$$

with

$$\alpha_j \equiv \begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ \alpha_{21}^j & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \alpha_{G1}^j & \dots & \dots & \dots & \alpha_{GG}^j \end{bmatrix} \quad (9b)$$

for regions with fission or upscattering. For regions without fission or upscatter, one can show

$$\alpha_j \equiv \begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ \alpha_{21}^j & 1 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 1 & 0 \\ \alpha_{G1}^j & \dots & \dots & \dots & 1 \end{bmatrix}. \quad (10a)$$

In addition in Eq.(9a)

$$h_j^\pm(x) \equiv \begin{bmatrix} h_{j1}^\pm(x) & 0 & \dots & 0 \\ 0 & h_{j2}^\pm(x) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & h_{jG}^\pm(x) \end{bmatrix} \quad (10b)$$

$$\mathbf{C}_{j1}^\pm \equiv \begin{bmatrix} C_{j11}^\pm \\ C_{j12}^\pm \\ \dots \\ C_{j1G}^\pm \end{bmatrix}. \quad (10c)$$

The final step is to find the coefficient vectors \mathbf{C}_{j1}^\pm .

3.2 . Initial form of the general solution

To determine \mathbf{C}_{j1}^\pm , we write the general solution in the following form assuming we know the particular solution $\phi_{pj}(x)$ and the boundary fluxes to give

$$\begin{aligned} \phi_j(x) &= \\ &= \left[\alpha_j h_j^+(x) \alpha_j^{-1} \right] (\phi_j - \phi_{pj}^+) + \\ &+ \left[\alpha_j h_j^-(x) \alpha_j^{-1} \right] (\phi_{j-1} - \phi_{pj}^-) + \phi_{pj}(x) \end{aligned} \quad (11a)$$

with

$$\phi_{pj}^+ \equiv \phi_{pj}(x_j), \quad \phi_{pj}^- \equiv \phi_{pj}(x_{j-1}).$$

For later use let

$$\begin{aligned} \mathbf{A}_j(x) &\equiv \alpha_j h_j^+(x) \alpha_j^{-1} \\ \mathbf{B}_j(x) &\equiv \alpha_j h_j^-(x) \alpha_j^{-1} \end{aligned} \quad (11b)$$

to give

$$\begin{aligned} \phi_j(x) &= \mathbf{A}_j(x) (\phi_j - \phi_{pj}^+) + \\ &\mathbf{B}_j(x) (\phi_{j-1} - \phi_{pj}^-) + \phi_{pj}(x). \end{aligned} \quad (11c)$$

Thus, we have formed a multigroup solution resembling that of the one-group case.

3.3. Determination of the interfacial boundary fluxes

We find the interfacial boundary fluxes from the following interfacial current continuity condition:

$$\begin{aligned} -\mathbf{D}_{j-1} \frac{d\phi_{j-1}(x)}{dx} \Big|_{x_{j-1}} &= \\ = -\mathbf{D}_j \frac{d\phi_j(x)}{dx} \Big|_{x_{j-1}}, \quad 2 \leq j \leq n \end{aligned}$$

When we introduce Eq.(11c) into this expression, a three-term recurrence relation results for the unknown interfacial fluxes

$$\begin{aligned} \mathbf{M}_j \boldsymbol{\phi}_j - \mathbf{N}_j \boldsymbol{\phi}_{j-1} - \mathbf{P}_j \boldsymbol{\phi}_{j-2} &= \\ &= \mathbf{f}_j, \quad 2 \leq j \leq n \end{aligned} \quad (12a)$$

and (after some algebra) we find

$$\begin{aligned} \mathbf{M}_j &\equiv \mathbf{D}_j \left. \frac{d\mathbf{A}_j(x)}{dx} \right|_{x_{j-1}} \\ \mathbf{N}_j &\equiv \mathbf{D}_{j-1} \left. \frac{d\mathbf{A}_{j-1}(x)}{dx} \right|_{x_{j-1}} - \mathbf{D}_j \left. \frac{d\mathbf{B}_j(x)}{dx} \right|_{x_{j-1}} \\ \mathbf{P}_j &\equiv \mathbf{D}_{j-1} \left. \frac{d\mathbf{B}_{j-1}(x)}{dx} \right|_{x_{j-1}} \end{aligned} \quad (12b)$$

$$\begin{aligned} \mathbf{f}_j &\equiv \mathbf{D}_j \left[\left. \frac{d\mathbf{A}_j(x)}{dx} \right|_{x_{j-1}} \boldsymbol{\phi}_{pj}^+ + \left. \frac{d\mathbf{B}_j(x)}{dx} \right|_{x_{j-1}} \boldsymbol{\phi}_{pj}^- - \left. \frac{d\boldsymbol{\phi}_{pj}(x)}{dx} \right|_{x_{j-1}} \right] - \\ &- \mathbf{D}_{j-1} \left[\left. \frac{d\mathbf{A}_{j-1}(x)}{dx} \right|_{x_{j-1}} \boldsymbol{\phi}_{pj-1}^+ + \left. \frac{d\mathbf{B}_{j-1}(x)}{dx} \right|_{x_{j-1}} \boldsymbol{\phi}_{pj-1}^- - \left. \frac{d\boldsymbol{\phi}_{pj-1}(x)}{dx} \right|_{x_{j-1}} \right] \end{aligned} \quad (12c)$$

For zero flux at the free surfaces, the recurrence naturally closes with

$$\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \mathbf{0}. \quad (12d)$$

We also impose this condition for zero currents at the free surfaces with appropriate modification of the coefficients of the first and last recurrence equations of Eqs.(12a).

3.4. The particular solution

The determination of the particular solution follows the standard method of variation of parameters for a vector solution to a second order ODE to give

$$\begin{aligned} \boldsymbol{\phi}_{pj}(x) &= \\ &= \boldsymbol{\alpha}_j \mathbf{h}_j^+(x) \int_x^{x_j} dx' \mathbf{h}_j^-(x') \mathbf{W}_j^{-1} \boldsymbol{\alpha}_j^{-1} \mathbf{q}_j(x') + \\ &\quad + \boldsymbol{\alpha}_j \mathbf{h}_j^-(x) \int_{x_{j-1}}^x dx' \mathbf{h}_j^+(x') \mathbf{W}_j^{-1} \boldsymbol{\alpha}_j^{-1} \mathbf{q}_j(x'), \end{aligned} \quad (13a)$$

with

$$\mathbf{W}_j^{-1} \equiv \text{diag} \left\{ \frac{B_{jk}}{\sin(B_{jk} \Delta_j)} \right\}.$$

Note that the particular solution has been constructed such that

$$\begin{aligned} \boldsymbol{\phi}_{pj}^+ &\equiv \boldsymbol{\phi}_{pj}(x_j) = \mathbf{0} \\ \boldsymbol{\phi}_{pj}^- &\equiv \boldsymbol{\phi}_{pj}(x_{j-1}) = \mathbf{0} \end{aligned} \quad (13b)$$

which simplifies Eq.(11a) to

$$\begin{aligned} \boldsymbol{\phi}_j(x) &= \left[\boldsymbol{\alpha}_j \mathbf{h}_j^+(x) \boldsymbol{\alpha}_j^{-1} \right] \boldsymbol{\phi}_j + \\ &+ \left[\boldsymbol{\alpha}_j \mathbf{h}_j^-(x) \boldsymbol{\alpha}_j^{-1} \right] \boldsymbol{\phi}_{j-1} + \boldsymbol{\phi}_{pj}(x) \end{aligned} \quad (14)$$

4. The recurrence relation and criticality

4.1. Final solution representation for $\boldsymbol{\phi}_j$

In accordance with solutions to 3-point recurrence relation of Eq.(12a), the interfacial flux is

$$\boldsymbol{\phi}_j = \mathbf{g}_j \boldsymbol{\phi}_0 + \boldsymbol{\rho}_j \boldsymbol{\phi}_1 + \mathbf{f}_{pj}, \quad (15)$$

where $\mathbf{g}_j, \boldsymbol{\rho}_j$ satisfy the homogeneous difference equation and \mathbf{f}_{pj} is a particular solution (not found here). Since, $\boldsymbol{\phi}_0 = \boldsymbol{\phi}_n = \mathbf{0}$, we have

$$\rho_n \phi = -f_{pj}. \quad (16)$$

Therefore, provided the inverse of ρ_n exists (which we shall consider below)

$$\phi = -\rho_n^{-1} f_{pj}, \quad (17)$$

and the general solution to the recurrence is

$$\phi_j = [1 - \rho_j \rho_n^{-1}] f_{pj}. \quad (18)$$

4.2. Criticality condition

For criticality

$$f_{pj} \equiv 0$$

and Eq.(16) becomes

$$\rho_n \phi = 0.$$

Since ϕ must be a non-vanishing vector, ρ_n must be singular or

$$\text{Det}[\rho_n(k_{eff})] = 0, \quad (19)$$

where we have divided all fission cross sections by k_{eff} whose value is the largest that satisfies Eq.(19). The critical flux is the k -eigenvector of the homogeneous form of Eq.(12a) corresponding to k_{eff} .

To normalize the flux to the fission source, we divide the flux by the fission source F ,

$$F \equiv \frac{1}{k_{eff}} \sum_{j=1}^n \nu \Sigma_{fj}^T \int_{x_{j-1}}^{x_j} dx \phi_j(x), \quad (20a)$$

which becomes

$$F \equiv \frac{1}{k_{eff}} \sum_{j=1}^n \nu \Sigma_{fj}^T \left[\alpha_j H_j \alpha_j^{-1} [\phi_j + \phi_{j-1}] \right], \quad (20b)$$

with

$$H_j \equiv \text{diag} \left\{ \frac{1}{B_{jk}} \left[\frac{1 - \cos(B_{jk} \Delta_j)}{\sin(B_{jk} \Delta_j)} \right] \right\}.$$

5. A critical benchmark comparison

We now consider a critical benchmark comparison to demonstrate the analytical formulation.

5.1 Numerical implementation

Numerical implementation for the fully analytical nodal solution is quite straightforward, where the most elaborate computation involves the determination of the B^2 -eigenvalues. The QR algorithm, as coded in the **BALANC**, **ELMHES** and **HQR** routines from *Numerical Recipes* [Press, 1992], gives these eigenvalues. The most intensive computation is the solution of Eq.(19) for k_{eff} . We use a binary search with the root bracketing **ZBRAK** routine, again from *Numerical Recipes* [Press, 1992]. The iteration is converged to 10^{-15} relative error. Complex arithmetic is required only to evaluate the coefficients given by Eqs.(11b). These quantities must be real for the flux to be real. We do not presuppose this and therefore compliance serves as a computational check. We require a numerical algorithm for matrix inversion in turning the recurrences given by Eqs.(12). Standard LU decomposition coded in the **LUDCMP** and **LUBKSUB** routines for real and complex elements from *Numerical Recipes* [Press, 1992] are suitable. The final numerical algorithm is the block triagdiagonal algorithm, which we have based on the corresponding scalar solver.

5.2. Nodal/Nodal comparison

A 4-group/2-region reactor serves as an example [Parsons, Nigg, 1985(1)] to test the numerical implementation of the theory presented above in the

ADSMGCR code. Each region is 30.48cm in width. One is fueled and one is not. A vacuum boundary condition is imposed on the right free surface and a zero current is assumed at the center. The INL/Analytic Nodal Code (ANC) and ADSMGCR give identical k_{eff} 's to all digits quoted. We also compared k_{eff} to those of PEBBED [Gougar et al., 2005] and PDQ [Pfeiffer, 1971], which differed from the analytical as observed in Table 1. We also obtained identical fluxes from ADSMGCR and ANC as displayed in Fig. 1.

6. Final comments

We have derived a fully analytical solution to the multigroup diffusion equations for a heterogeneous medium. Muller [Muller, 1989] presented an almost identical approach but in a response matrix form. This may indeed be a more appropriated formulation, which we will investigate in a future effort. Finally, we mention that the above formulation is appropriate in 1D spherical and cylindrical geometries with a change to the appropriate solutions h_j^{\pm} of the 1D diffusion equation.

References

- D.K. Parsons and D. Nigg, EGG-PBS-6821 INEL Report, Oct. 1985(1).
D.K. Parsons and D. Nigg, *Trans., Am.Nucl. Soc.*, v50, 282-283, 1985(2).
M.M. Aburomia, BWR Refill-Reflood Program, TRAC-BWR, Component Development, NUREG/CR-2135 (EPRI NP-1583/GEAP-24941), Dec. 1981.
R.A. Shober, Nodal Method for Solving Transient Few-Group Neutron Diffusion Equations, ANL-78-51, 1978.
K. Smith, An Analytical Nodal Method for Solving the Two-Group, Multidimensional, Static and Transient Neutron Diffusion Equation, MS Thesis, MIT, 1979.
F. Press, et. al., *Numerical Recipes in FORTRAN: The Art of Scientific Computing*, 2nd ed., Cambridge Univ. Press., Boston, 1992.
H.D. Gougar, A.M. Ougouag, W.K. Terry, Validation of the Neutronic Solver within the PEBBED Code for Pebble Bed Reactor Design, *Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear*

and Biological Applications, Palais des Papes, Avignon, France, September 12-15, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

C.J. Pfeiffer, PDQ-7 Reference Manual II, WAPD-TM-947 (6), 1971.

E.Z. Müller, Environment-Insensitive Equivalent Diffusion Theory Group Constants for Pressurized Water Reactor Radial Reflector Regions, *Nuc. Sci.& Eng.*, 103, 359, 1989.

Table 1
 k_{eff} Comparison

Analytic Nodals	1.2463677
PDQ (80 nodes)	1.246 547
PDQ (160 nodes)	1.246 402
PDQ (320 nodes)	1.246365
PEBBED (Nodal)	1.2463 521
PEBBED (FD)	1.2463 026

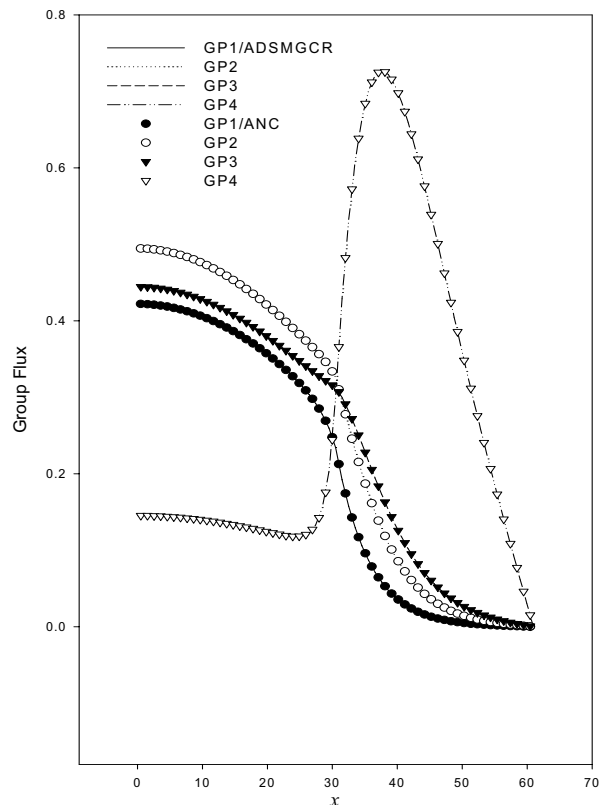


Fig. 1 Comparison of fluxes from ADSMGCR and INL/ANC